Contents

Reading:

1. Ch. 17, Ashcroft & Mermin
2. Chs. 5& 6, Kittel
3. For a more detailed discussion of Fermi liquid theory, see G. Baym and C. Pethick, Landau Fermi-Liquid Theory : Concepts and Applications, Wiley 1991

2 Electron-electron interactions

The electronic structure theory of metals, developed in the 1930's by Bloch, Bethe, Wilson and others, assumes that electron-electron interactions can be neglected, and that solid-state physics consists of computing and filling the electronic bands based on knowldege of crystal symmetry and atomic valence. To a remarkably large extent, this works. In simple compounds, whether a system is an insulator or a metal can be determined reliably by determining the band filling in a noninteracting calculation. Band gaps are sometimes difficult to calculate quantitatively, but inclusion of simple renormalizations to 1-electron band structure known as Hartree-Fock corrections, equivalent to calculating the average energy shift of a single electron in the presence of an average density determined by all other electrons ("mean field theory"), almost always suffices to fix this problem. There are two reasons why we now focus our attention on $e^- - e^-$ interactions, and why almost all problems of modern condensed matter physics as it relates to metallic systems focus on this topic:

1. Why does the theory work so well in simple systems? This is far from clear. In a good metal the average interelectron distance is of the order of or smaller than the range of the interaction, e.g. the screening length $\ell_{scr} \sim (c/e^2 m)^{1/2} \rho^{-1/6}$, where ρ is the density, of order 1nm for typical parameters. One might therefore expect that interactions should strongly modify the picture of free electrons commonly used to describe metals.

2. More complicated systems exhibit dramatic deviations from the predictions of band theory. I refer now not simply to large quantitative errors in the positions of 1-electron bands, but to qualitative discrepancies in the behavior of the materials. The most interesting modern example is the class of compounds known as the transition metal oxides, including the cuprate materials which give rise to high-temperature superconductivity (HTS).[1]

[1]The parent compounds of the HTS (e.g. La_2CuO_4 and $YBa_2Cu_3O_4$ are without exception *antiferromagnetic* and *insulating*. Historically, this discovery drove much of the fundamental interest in these materials, since standard electronic structure calculations predicted they should be paramagnetic metals. This can easily be seen by simple valence counting arguments. The nominal valences in e.g. La_2CuO_4 are La^{3+}, O^{2-}, and Cu^{2+} The La and O ions are in closed shell configurations, whereas the Cu is in an $[Ar]3d^9$ state, i.e. a single d-hole since

2.1 Mean field theory (Hartree-Fock)

Let's begin with the second-quantized form of the electronic Hamiltonian with 2-body interactions. The treatment will be similar to that of Kittel (Ch. 5), but for comparison I will focus on a translationally invariant system and do the calculation in momentum space. In this case as we have shown the Hamiltonian is[2]

$$
\begin{aligned}
\hat{H} &= \hat{T} + \hat{V}, & (1)\\
\hat{T} &= = \sum_{\mathbf{k}\sigma} \left(\frac{\mathbf{k}^2}{2m}\right) c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} & (2)\\
\hat{V} &= \frac{1}{2} \sum_{\substack{\mathbf{k},\mathbf{k}',\mathbf{q}\\ \sigma,\sigma'}} c^\dagger_{\mathbf{k}\sigma} c^\dagger_{\mathbf{k}'+\mathbf{q}\sigma'} V(\mathbf{q}) c_{\mathbf{k}'\sigma'} c_{\mathbf{k}+\mathbf{q}\sigma}. & (3)
\end{aligned}
$$

The 2-body interaction $\hat{V}$ contains 4 Fermi operators c and is therefore not exactly soluble. The goal is to write down an *effective* 2-body

there are 10 d electrons in a filled shell. The 1 hole/unit cell would then suggest a 1/2 filled band and therefore a metallic state. The crystal field splittings in the planar Cu environment give the $3d_{x^2-y^2}$ state being lowest in energy (see later), and since the n.n.'s are the $O's$, it would seem likely that the lowest O crystal field state in the planar environment, the O $3p$, will hybridize with it. Sophisticated LDA calculations confirm this general picture that the dominant band at the Fermi level is a 1/2-filled planar Cu $d_{x^2-y^2}$- O $3p$ band. Instead, this compound is found experimentally to be an electrical insulator and an antiferromagnet with a Neel temperature of 300K! This strongly suggests that the band calculations are missing an important element of the physics of the high-T_c materials. In the transition metals and TMO's band theory is notoriously bad at calculating band gaps in insulators, because of the presence of strong local Coulomb interactions which lead to electronic correlations neglected in the theory. It is therefore reasonable to assume that a similar mechanism may be at work here: extremely strong Coulomb interactions in the $Cu-O$ planes are actually opening up a gap in the 1/2-filled band at the Fermi level and simultaneously creating a magnetic state. This phenomenon has been studied in simpler systems since the 60s and is known as the *Mott-Hubbard* transition.

[2]For the moment, we ignore the ionic degrees of freedom and treat only the electrons. To maintain charge neutrality, we therefore assume the electrons move in a neutralizing positive background ("jellium model").

Hamiltonian which takes into account the average effects of the interactions. We therefore replace the 4-Fermi interaction with a sum of all possible 2-body terms,

$$c_1^\dagger c_2^\dagger c_3 c_4 \;\simeq\; -\langle c_1^\dagger c_3\rangle c_2^\dagger c_4 - \langle c_2^\dagger c_4\rangle c_1^\dagger c_3 + \langle c_1^\dagger c_4\rangle c_2^\dagger c_3 + \langle c_2^\dagger c_3\rangle c_1^\dagger c_4, \quad (4)$$

where the $+$ and $-$ signs are dictated by insisting that one factor of -1 occur for each commutation of two fermion operators required to achieve the given ordering. This can be thought of as "mean field terms", in the spirit of Pierre Weiss, who replaced the magnetic interaction term $S_i \cdot S_j$ in a ferromagnet by $\langle S_i\rangle S_j = \langle S\rangle S_j \equiv -H_{eff} S_j$, i.e. he replaced the field S_i by its homogeneous mean value S, and was left with a term equivalent to a 1-body term corresponding to a spin in an external field which was soluble. The mean field $\langle S\rangle$ in the Weiss theory is the instantaneous average magnetization of all the other spins except the spin S_j, and here we attempt the same thing, albeit somewhat more formally. The "mean field"

$$\langle c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}'\sigma'}\rangle = \langle c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma}\rangle \delta_{\mathbf{k}\mathbf{k}'}\delta_{\sigma\sigma'} \equiv n_{\mathbf{k}\sigma}\delta_{\mathbf{k}\mathbf{k}'}\delta_{\sigma\sigma'} \quad (5)$$

is the average number of particles $n_{\mathbf{k}\sigma}$ in the state $\mathbf{k}\sigma$, which will be weighted with the 2-body interaction $V(\mathbf{q})$ to give the average interaction due to all other particles (see below).[3]

[3]Note we have not allowed for mean fields of the form $\langle c^\dagger c^\dagger\rangle$ or $\langle aa\rangle$. These averages vanish in a normal metal due to number conservation, but will be retained in the theory of superconductivity.

With these arguments in mind, we use the approximate form (4) and replace the interaction $\hat{V}$ in (3) by

$$\begin{aligned}
\hat{V}_{HF} &= \frac{1}{2} \sum_{\substack{\mathbf{k}\mathbf{k}'\mathbf{q} \\ \sigma\sigma'}} V(\mathbf{q}) \Big[-\langle c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}'\sigma'} \rangle c^\dagger_{\mathbf{k}'+\mathbf{q}\sigma'} c_{\mathbf{k}+\mathbf{q}\sigma} - \langle c^\dagger_{\mathbf{k}'+\mathbf{q}\sigma'} c_{\mathbf{k}+\mathbf{q}\sigma} \rangle c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}'\sigma'} + \\
&\quad + \langle c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}+\mathbf{q}\sigma} \rangle c^\dagger_{\mathbf{k}'+\mathbf{q}\sigma'} c_{\mathbf{k}'\sigma'} + \langle c^\dagger_{\mathbf{k}'+\mathbf{q}\sigma'} c_{\mathbf{k}'\sigma'} \rangle c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}+\mathbf{q}\sigma} \Big] \\
&= -\sum_{\substack{\mathbf{k}\mathbf{q} \\ \sigma}} V(\mathbf{q}) \langle c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} \rangle c^\dagger_{\mathbf{k}+\mathbf{q}\sigma} c_{\mathbf{k}+\mathbf{q}\sigma} + V(0) \sum_{\substack{\mathbf{k}\mathbf{k}' \\ \sigma\sigma'}} \langle c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} \rangle c^\dagger_{\mathbf{k}'\sigma'} c_{\mathbf{k}'\sigma'} \\
&= \sum_{\mathbf{k}\sigma} \left(-\sum_{\mathbf{q}} n_{\mathbf{k}-\mathbf{q}\sigma} V(\mathbf{q}) + nV(0) \right) c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}, \qquad (6)
\end{aligned}$$

where the total density n is defined to be $n = \Sigma_{\mathbf{k}\sigma} n_{\mathbf{k}\sigma}$. Since this is now a 1-body term of the form $\Sigma_{\mathbf{k}\sigma} \Sigma_{HF}(\mathbf{k}) a^\dagger_{\mathbf{k}\sigma} a_{\mathbf{k}\sigma}$, it is clear the full Hartree-Fock Hamiltonian may be written in terms of a $\mathbf{k}$-dependent energy *shift*:

$$\hat{H}_{HF} = \sum_{\mathbf{k}\sigma} \left(\frac{\hbar^2 k^2}{2m} + \Sigma_{HF}(\mathbf{k}) \right) c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}, \qquad (7)$$

$$\Sigma_{HF}(\mathbf{k}) = \underbrace{-\sum_{\mathbf{q}} n_{\mathbf{k}-\mathbf{q}\sigma} V(\mathbf{q})}_{Fock} + \underbrace{nV(0)}_{Hartree} \qquad (8), (9)$$

Note the Hartree or *direct Coulomb* term, which represents the average interaction energy of the electron $\mathbf{k}\sigma$ with all the other electrons in the system, is merely a constant, and as such it can be absorbed into a chemical potential. In fact it is seen to be divergent if $V(q)$ represents the Coulomb interaction $4\pi e^2/q^2$, but this divergence must cancel exactly with the constant arising from the sum of the self-energy of the positive background and the interaction energy of the electron gas with that background.[4] The Fock, or *exchange* term[5] is a momentum-dependent shift.

2.1.1 Validity of Hartree-Fock theory

Crucial question: when is such an approximation a good one for an interacting system? The answer, curiously, turns out to be different for bosons and fermions. The HF approximation is a good one for interacting *low density Bose systems* or *high density Fermi systems*!

Intuitively it seems obvious that if the particles are further apart on the average, they will interact less strongly and less often, so a mean field theory like Hartree-Fock theory should work well. This is true in the Bose case: the only characteristic energies are the temperature T and the zero-point energy. The latter is just the energy scale obtained by confining the particle to a cage of size the interparticle spacing r_s, i.e. $\hbar^2/(2mr_s^2)$. The interaction is typically characterized by a *strength* V and a *range* a, and if $r_s \gg a$, the particles don't feel the potential much and the ground state energy, for example, of such a gas can be expanded

[4] See e.g., Kittel

[5] The origin of the term exchange is most easily seen in many-body perturbation theory, where the Fock term is seen to arise from a scattering process where the particle in state $\mathbf{k}\sigma$ changes places with a particle from the medium in an intermediate state.

at $T = 0$ in powers of a/r_s. The result is

$$E_0 = E_0^{HF} + E_{corr} \tag{10}$$

with E_0^{HF} the ground state energy calculated in the independent particle approximation with the Hartree-Fock energy shifts, and E_{corr} the *correlation energy*, which is found to vary as

$$\frac{E_{corr}}{E_0^{HF}} \simeq \frac{1}{r_s^\alpha}, \text{ (bosons)} \tag{11}$$

with $\alpha = xxx$, and therefore $\to 0$ in the low density limit.

In the case of Fermions, a new energy scale arises due to the Pauli principle, namely ε_F. As the density increases, so does ε_F, which represents the average kinetic energy of electrons; this increase is faster than the increase of the correlation energy. For the electron gas with Coulomb interactions, for example, we have, in terms of the Bohr radius a_0 we have (per particle)

$$K.E. = \tfrac{3}{5}\varepsilon_F = \frac{2.21}{r_s^2} \text{ Ryd} \tag{12}$$

$$P.E.|_{HF} = \frac{-0.916}{r_s} \text{ Ryd} \tag{13}$$

and the correlation energy is given by

$$\frac{E_{corr}}{\text{Ryd}} = 0.0622 \log r_s - 0.096 + \ldots \tag{14}$$

so it is clear the correlation term is less singular than the HF term in the limit $r_s \to 0$. At higher densities, particles are effectively independent.[6]

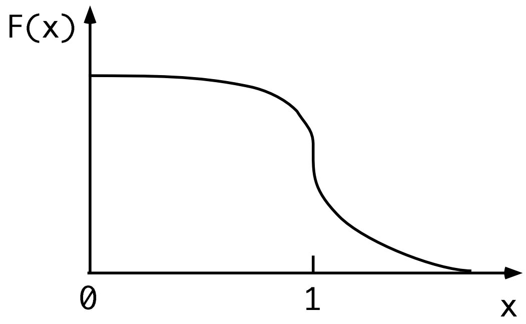
[6]For a more detailed discus of these terms, see Fetter & Wallecka, *Quantum Theory of Many-Particle Systems*

2.1.2 Problem with Hartree-Fock theory

Although we argued that the Hartree-Fock approximation becomes a better approximation in the limit of low (high) density for bosons (fermions), it never becomes exact, as one can see by examining the Fourier transform of the Hartree-Fock energy shift in the presence of the bare Coulomb interaction $V(\mathbf{q}) = 4\pi e^2/q^2$. The Hartree term itself (being $\mathbf{k}$ independent) is absorbed into a redefinition of the chemical potential, so the shift is (T=0):

$$\delta\varepsilon_{\mathbf{k}} = \pm\frac{1}{L^3}\sum_{|\mathbf{k}'|<k_F}\frac{4\pi e^2}{|\mathbf{k}-\mathbf{k}'|^2} \quad (15)$$

$$= \frac{2e^2 k_F}{\pi}F(k/k_F), \quad (16)$$



where $F(x)$ is a function which has a log divergence in slope at $x = 1$, i.e. at the Fermi level.[7] This means while the energy *shift* might be small compared to the Fermi energy $\mathbf{v}\varepsilon_F$, the *velocity* of an electron is $\partial\varepsilon_{\mathbf{k}}/\partial\mathbf{k}|_{k_F}$, which contains a term which is infinite.

[7]The integral is straightforward & useful:

$$\frac{1}{L^3}\sum_{\mathbf{k}'}{}' \frac{1}{(\mathbf{k}-\mathbf{k}')^2} = \int_0^{k_F}\frac{k^2dk}{4\pi^2}\int_{-1}^{1}dx\frac{1}{k^2-k'^2-2kk'x} = \frac{1}{8\pi^2 k}\int_0^{k_F}dk'\,k'\,\log\left|\frac{k+k'}{k-k'}\right| \quad (17)$$

$$= \frac{1}{8\pi^2}\left(\frac{k_F^2-k^2}{k}\log\left|\frac{k_F+k}{k_F-k}\right| + 2k_F\right) \quad (18)$$

so with $z = k/k_F$ and (16) we have

$$\boxed{F(z) = \frac{1-z^2}{4z}\log\left|\frac{1+z}{1-z}\right| + \frac{1}{2}} \quad (19)$$

This problem can be traced back to the long-range nature of the Coulomb force. Two electrons at large distances $\mathbf{r}-\mathbf{r}'$ don't really feel the full $1/|\mathbf{r}-\mathbf{r}'|^2$ but a "screened" version due to the presence of the intervening medium, i.e. The electron gas rearranges itself to cancel out the long-range part of V.

2.2 Screening

2.2.1 Elementary treatment

To see how this works, let's first examine the problem of a single fixed (i.e. infinite mass) charge placed inside an electron gas. We are interested in how the electron gas responds to this perturbation (recall in the HF approximation the perturbation would simply be the interaction of the charge with the uniform gas). But since the electrons are mobile and negatively charged, they will tend to cluster around the test charge if its charge is positive, and be repelled (i.e. have a lower density) around the test charge if it is negative. In addition, Fermi statistics lead to long-range *oscillations* of the electron charge density far from the test charge.

This is not entirely a "Gedanken experiment". Impurities in solids may have different valences from the host, and thus acquire a localized charge, although the entire solid is still neutral. As an example of some relevance to modern condensed matter physics, consider what happens when you put an extra Oxygen atom in the CuO_2 plane of a cuprate high-T_c superconducting material. Although the crystal structure of these materials is complex, they all contain CuO_2 planes as shown in the figures. The interstitial oxygen will capture two electrons from the valence band, changing it from a $2s^22p^4$ to a $2s^22p^6$ electronic configuration. The impurity will then have a net charge of two electrons.

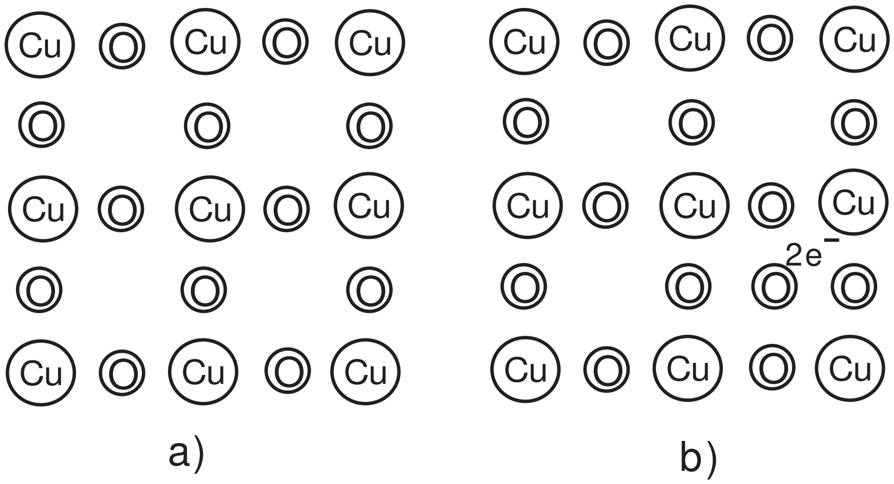


Figure 1: *a) The CuO_2 plane of cuprate superconductor. b) Interstitial charged O impurity.*

Near the impurity, the electronic charge density will be reduced by the Coulomb interaction. Near the impurity (since the electrostatic potential $e\delta\phi(\mathbf{r}_{imp}) < 0$ with $e > 0$)

$$n(\mathbf{r}_{imp}) \approx \int_{-e\delta\phi(\mathbf{r}_{imp})}^{\varepsilon_F} N(\omega)d\omega \approx \int_0^{\varepsilon_F + e\delta\phi(\mathbf{r}_{imp})} N(\omega')d\omega' \qquad (20)$$

Note that this equation involves the double-spin density of states, which we will use throughout this section. On the other hand, in bulk far away

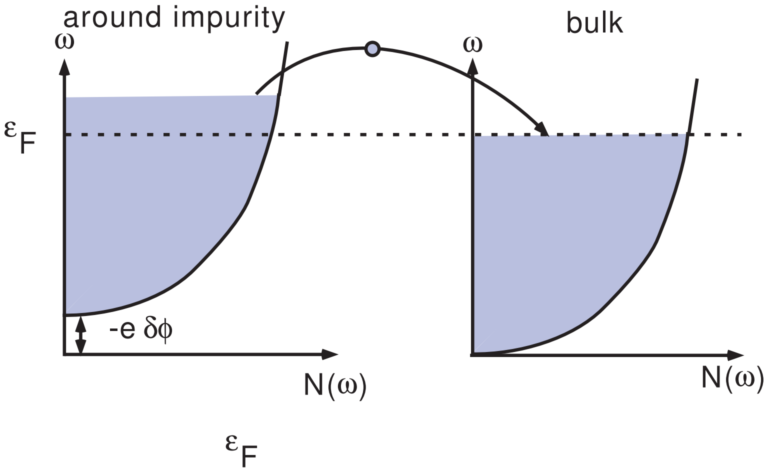


Figure 2: *Local repulsion of charge due to shift of electronic density of states near impurity*

from the impurity, $\delta\phi(\mathbf{r}_{bulk}) = 0$, so

$$n(\mathbf{r}_{bulk}) \approx \int_0^{\varepsilon_F} N(\omega)d\omega \tag{21}$$

or

$$\delta n(\mathbf{r}) \approx \int_0^{\varepsilon_F + e\delta\phi(\mathbf{r})} N(\omega)d\omega - \int_0^{\varepsilon_F} N(\omega)d\omega \tag{22}$$

Let us assume a *weak potential* $|e\delta\phi| \ll \varepsilon_F$; therefore

$$\delta n(\mathbf{r}) \approx N(\varepsilon_F)\left[\varepsilon_F + e\delta\phi - \varepsilon_F\right] = e\delta\phi N(\varepsilon_F)\,. \tag{23}$$

We can solve for the change in the electrostatic potential by solving Poisson equation.

$$\nabla^2\delta\phi = 4\pi\delta\rho = -4\pi e\delta n = -4\pi e^2 N_0\delta\phi\,. \tag{24}$$

Define a new length k_{TF}^{-1}, the Thomas-Fermi screening length, by $k_{TF}^2 = 4\pi e^2 N_0$, so that P's eqn. may be written $\nabla^2\delta\phi = k_{TF}^2\delta\phi$, which has the solution $\delta\phi(\mathbf{r}) = C\exp(-k_{TF}r)/r$. Now C may be deterined by letting $N(\varepsilon_F) = 0$, so the medium in which the charge is embedded becomes vacuum. Then the potential of the charge has to approach q/r, so $C = q$, i.e. in the electron gas

$$\delta\phi(\mathbf{r}) = \frac{qe^{-k_{TF}r}}{r}. \tag{25}$$

Let's estimate some numbers, by using the free electron gas. Use $k_F = (3\pi^2 n)^{1/3}$, $a_0 = \hbar^2/(me^2) = 0.53\mathring{\mathrm{A}}$, and $N(\varepsilon_F) = mk_F/(\hbar^2\pi^2)$. Then we find

$$\begin{aligned} k_{TF}^{-2} &= \frac{a_0\pi}{4(3\pi^2 n)^{1/3}} \approx \frac{a_0}{4n^{1/3}} \\ k_{TF}^{-1} &\approx \frac{1}{2}\left(\frac{n}{a_0^3}\right)^{-1/6} \end{aligned} \tag{26}$$

In Cu, for which $n \approx 10^{23}$ cm^{-3} (and since $a_0 = 0.53\mathring{\mathrm{A}}$)

$$k_{TF}^{-1} \approx \frac{1}{2}\frac{\left(10^{23}\right)^{-1/6}}{\left(0.5\times10^{-8}\right)^{-1/2}} \approx 0.5\times10^{-8}\ \mathrm{cm}\ = 0.5\mathring{\mathrm{A}} \tag{27}$$

Thus, if we add a charged impurity to Cu metal, the effect of the impurity's ionic potential is exponentially screened away for distances $r > \frac{1}{2}\mathring{\mathrm{A}}$. The screening length in a semiconductor can clearly be considerably longer because n is much smaller, but because of the 1/6 power which appears in, even with $n = 10^{-10}$, k_{TF}^{-1} is only about 150 times larger or $75\mathring{\mathrm{A}}$.

What happens in the quantum-mechanical problem of an electron moving in the potential created by the impurity when the screening

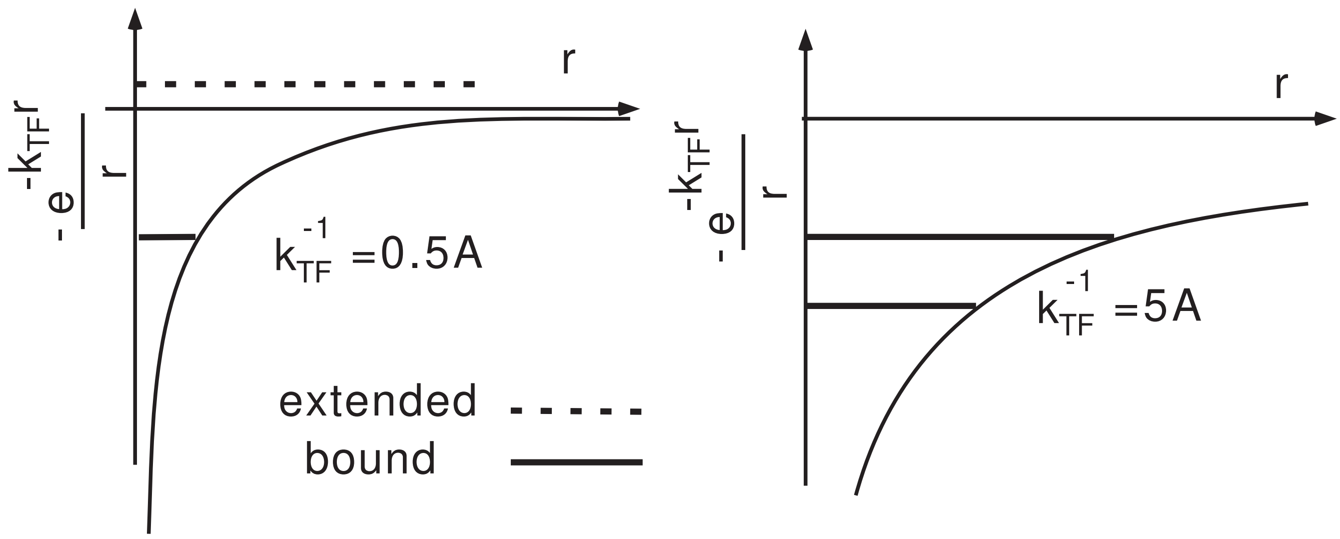


Figure 3: *Screened impurity potentials. As the density decreases, the screening length increases, so that states which were extended bound.*

length gets long? As shown in the figure, the potential then correspondingly deepens, and from elementary quantum mechanics we expect it to be able to bind more electrons, i.e bound states "pop out" of the continuum into orbits bound to the impurity site.

In a poor metal (e.g., YBCO), in which the valence state is just barely unbound, decreasing the number of carriers will increase the screening length, since

$$k_{TF}^{-1} \sim n^{-1/6} \,. \tag{28}$$

This will extend the range of the potential, causing it to trap or bind more states–making the one free valence state bound. Of course, this has only a small effect $\mathcal{O}(1/N)$ effect on the bulk electrical properties of the material. Now imagine that instead of a single impurity, we have a concentrated system of such ions, and suppose that we decrease n (e.g. in Si-based semiconductors, this is done by adding acceptor dopants, such as B, Al, Ga, etc.). This will in turn, increase the screening length, causing some states that were free to become bound, eventually possibly causing an abrupt transition from a metal to an insulator. This process is believed to explain the metal-insulator transition in some amorphous semiconductors.

2.2.2 Kubo formula

Many simple measurements on bulk statistical systems can be described by applying a small external probe field of some type to the system at $t = 0$, and asking how the system responds. If the field is small enough, the response is proportional to the external perturbation, and the proportionality constant, a *linear response coefficient*, is given always in terms of a *correlation function* of the system in the equilibrium ensemble without the perturbation. In Table 1 I list some standard linear response coefficients for condensed matter systems.

System	Perturbation	Response	Coefficient
metal	electric field $\mathbf{E}$	current $\mathbf{j}$	conductivity σ
	temp. gradient ∇T	heat current $\mathbf{j}_Q$	thermal cond. κ
	point charge q	density fluct. δn	density correlation function χ_c
	magnetic field B	magnetization M	susceptibility χ_s

The general theory of linear response is embodied in the *Kubo formula*.[8] Suppose a perturbation $\hat{H}'(t)$ is turned on at time $t = 0$. The idea is to express the subsequent time-dependence of expectation values of physical observables in terms of matrix elements of the perturbation *in the unperturbed ensemble.* The unperturbed ensemble is described by $\hat{H}_0$, which may involve interactions, but is usually assumed to be time-independent. All observables can be calculated by knowing the time evolution of the statistical operator $\rho(t)$, given by the Heisenberg equation

$$i\frac{\partial\hat{\rho}}{\partial t} = [\hat{H}_0 + \hat{H}', \hat{\rho}] \tag{29}$$

First one defines a canonical transformation[9]:

$$\tilde{\rho}(t) = \hat{S}(t)\hat{\rho}(t)\hat{S}^\dagger; \quad S(t) \equiv e^{i\hat{H}_0 t} \tag{30}$$

[8] R. Kubo, J. Phys. Soc. Jpn. 12, 570 (1957).

[9] The idea is to remove the "trivial" time-evolution of $\hat{\rho}$ on $\hat{H}$, to isolate the dependence on $\hat{H}'$.

from which one can see by substituting into (29) that

$$i\frac{\partial\tilde{\rho}}{\partial t} = [\tilde{H}', \tilde{\rho}] \tag{31}$$

with $\tilde{H}' = \hat{S}\hat{H}'\hat{S}^\dagger$. This has the formal solution

$$\tilde{\rho}(t) = \tilde{\rho}(0) - i\int_0^t [\tilde{H}', \tilde{\rho}(0)]dt'. \tag{32}$$

The initial condition is $\tilde{\rho}(0) = \hat{S}(0)\hat{\rho}(0)\hat{S}(0)^\dagger = \hat{\rho}(0)$, and we can iterate the rhs by substituting $\hat{\rho}(0)$ for $\tilde{\rho}(0)$, etc.[10] Since we are interested only in leading order, we write

$$\tilde{\rho}(t) \simeq \hat{\rho}(0) - i\int_0^t [\tilde{H}', \hat{\rho}(0)]dt'. \tag{33}$$

If we now multiply on the left by $\hat{S}^\dagger$ and on the right by $\hat{S}$, we obtain the leading order in $\hat{H}'$ change in the original ρ:

$$\hat{\rho}(t) \simeq \hat{\rho}(0) - i\hat{S}^\dagger(t)\left\{\int_0^t [\tilde{H}', \hat{\rho}(0)]dt'\right\}\hat{S}(t), \tag{34}$$

which can now be used to construct averages in the usual way. The expectation value of an operator $\hat{\mathcal{O}}$ at nonzero T and at some time t is

$$\begin{aligned}
\langle\hat{\mathcal{O}}\rangle &\equiv \mathrm{Tr}(\hat{\rho}(t)\hat{\mathcal{O}}) && (35)\\
&\simeq \mathrm{Tr}\left(\hat{\rho}(0)\hat{\mathcal{O}}\right) - i\int dt'\mathrm{Tr}\left(S^\dagger(t)[\tilde{H}', \hat{\rho}(0)]\hat{S}(t)\hat{O}\right)\\
&= \mathrm{Tr}\left(\hat{\rho}(0)\hat{\mathcal{O}}\right) - i\int dt'\mathrm{Tr}\left(\hat{\rho}(0)[\tilde{H}', \hat{\mathcal{O}}_H(t)]\right), && (36)
\end{aligned}$$

[10] Note $\hat{\rho}(0)$ is the unperturbed but still interacting density matrix (statistical operator). I reserve the symbol $\hat{\rho}_0$ for the noninteracting analog.

where in the last step the cyclic property of the trace and the definition of the Heisenberg operator $\hat{O}_H = \hat{S}\hat{\mathcal{O}}\hat{S}^\dagger$ was used. The change in the expectation value due to the perturbation is then

$$\boxed{\delta\langle\hat{\mathcal{O}}\rangle = -i\int dt'\mathrm{Tr}\left(\hat{\rho}(0)[\tilde{H}', \hat{\mathcal{O}}_H(t)]\right)} \tag{37}$$

Since typically $\hat{H}'$ is proportional to some external (c-number) field, we can write $\hat{H}'$ as $\hat{H}'(t) = \int d^3r\hat{B}(\mathbf{r})\phi(\mathbf{r},t)$ (so $\tilde{\hat{H}}'(t) = \int d^3r\hat{B}_H(\mathbf{r},t)\phi(\mathbf{r},t)$), and

$$\begin{aligned}\delta\langle\hat{A}(1)\rangle &= -i\int_0^t\int \mathrm{Tr}\left(\hat{\rho}(0)[\hat{A}_H(1), \hat{B}_H(1')]\right)\phi(1')d1' &(38)\\ &\equiv \int_0^\infty G_{AB}(1,1')\phi(1')d1'. &(39)\end{aligned}$$

with the notation $1 \equiv \mathbf{r}, t, \sigma$, $1' = \mathbf{r}', t', \sigma'$, $\int d1' \equiv \sum_{\sigma'}\int d^3r'dt'$, etc.[11]

2.2.3 Correlation functions

As a concrete example, consider the change in the density $\delta n(\mathbf{r},t)$ of a system in response to a local change in its density perhaps at a different place and time $\delta n(\mathbf{r}',t')$, where $\hat{n}(\mathbf{r}) = \langle\hat{\psi}^\dagger(\mathbf{r})\hat{\psi}(\mathbf{r})\rangle$, and $\langle\hat{\psi}^\dagger(\mathbf{r})\hat{\psi}(\mathbf{r})\rangle_{\hat{H}'=0} = n_0$. It's usually convenient to set $n_0 = 0$, i.e. we assume an overall neutral system. The linear response function is then

$$\chi(\mathbf{r},t;\mathbf{r}',t') = -i\langle[\hat{n}(\mathbf{r},t), \hat{n}(\mathbf{r}',t')]\rangle_{\hat{H}'=0}\theta(t-t'), \tag{40}$$

[11] The object $\mathrm{Tr}\left(\hat{\rho}(0)[\hat{A}_H(1), \hat{B}_H(1')]\right)$ which appears on the right-hand side of (37) is related to something called a retarded 2-particle Green's function, which I have promised not to oppress you with.

where the exectation value is taken in the unperturbed system. The function G_{nn} measures the average amplitude in the unperturbed ensemble a particle is to be found at $\mathbf{r}', t'$ and subsequently at $\mathbf{r}, t$. If the particles are statistically independent, χ factorizes, $\langle nn' \rangle \sim \langle n \rangle \langle n' \rangle = 0$ (no *correlations*), so it has the interpretation of a *correlation function.*

2.2.4 Dielectric constant

The simplest way to analyze this problem conceptually is to ask what is the potential a long distance from a test charge placed into the interacting electron gas medium. This potential will be the sum of the bare potential produced by the test charge in a vacuum, plus the induced potential due to the polarization of the medium.

Let's use what we learned about linear response in the last section to calculate the electric potential in the system $\phi(\mathbf{r}, t)$ due to an *external* potential $\phi^{ext}(\mathbf{r}', t')$ (you may think of this as the potential due to a test charge if you like). From electrodynamics we recall these two are supposed to be proportional, and that the proportionality constant is just the dielectric constant ϵ. By analogy we write, in Fourier transformed language,

$$\phi^{ext}(\mathbf{q}, \omega) = \epsilon(\mathbf{q}, \omega)\phi(\mathbf{q}, \omega) \tag{41}$$

It is the dielectric constant of the medium (which is directly related to the conductivity) which we now wish to calculate.

The total potential in the material is the sum of the external potential and the induced potential,

$$\phi = \phi^{ind} + \phi^{ext}, \tag{42}$$

but in fact we can calculate the induced potential ϕ^{ind} by

- first finding the induced change in density $\delta\rho^{ind}$ due to the external potential, using linear response theory; then
- using Poisson's equation to calculate the induced electric potential.

The additional term in the Hamiltonian in the presence of the "test charge" is

$$\hat{H}' = e \int d^3r \; \hat{n}(\mathbf{r})\phi(\mathbf{r}, t) \tag{43}$$

where $\hat{n}$ is the 2nd-quantized density operator $\hat{\psi}^\dagger\hat{\psi}$. The induced change in charge density $\delta\rho = e\langle\hat{n}\rangle$ is then just given by the Kubo formula as above,[12]

$$\begin{aligned} \delta\rho^{ind}(1) &= -ie^2 \int_0^t \int d^3r' \mathrm{Tr}\left(\hat{\rho}(0)[\hat{n}_H(1), \hat{n}_H(1')]\right)\phi^{ext}(1')d1' & (44) \\ &\equiv e^2 \int_0^\infty \chi(1, 1')\phi^{ext}(1')d1' & (45) \end{aligned}$$

where the density-density correlation function is[13]

$$\chi(1, 1') = -i\mathrm{Tr}\left(\hat{\rho}(0)[\hat{n}_H(1), \hat{n}_H(1')]\right)\theta(t - t'). \tag{46}$$

[12] Don't confuse charge density ρ with statistical operator $\hat{\rho}$.

[13] Instead of $G^{(2)}_{nn}$, it's more conventional to use the notation χ_{nn} or just χ.

For a translationally invariant system in Fourier transform rep., the convolution (45) reduces to

$$\delta\rho^{ind}(\mathbf{q},\omega) = e^2\chi(\mathbf{q},\omega)\phi^{ext}(q,\omega). \tag{47}$$

Now using Poisson's equation $q^2\phi^{ind} = 4\pi\delta\rho^{ind}$, and Eq. (42), we find[14]

$$\phi^{ind}(\mathbf{q},\omega) = \frac{4\pi e^2}{q^2}\chi(\mathbf{q},\omega)\phi^{ext}(\mathbf{q},\omega) \equiv V(\mathbf{q})\chi(\mathbf{q},\omega)\phi^{ext} \tag{48}$$

so

$$\boxed{\epsilon(\mathbf{q},\omega) \equiv \frac{\phi^{ext}(\mathbf{q},\omega)}{\phi^{ind}(\mathbf{q},\omega)+\phi^{ext}(\mathbf{q},\omega)} = \frac{1}{1+V(\mathbf{q})\chi(\mathbf{q},\omega)}.} \tag{49}$$

2.2.5 Lindhard function

We've found the exact structure of the dielectric response,[15] but not really solved it because we still don't know the density-density correlation function χ. For the interacting system this can be a very difficult problem, but it is not too hard to find it for the free fermion gas. We will need

[14] Compare Eq. (24)

[15] Warning! Compare the treatment here with e.g., A& M pp. 337-340, and you will see that they arrive at the apparently different result

$$\epsilon(\mathbf{q},\omega) = 1 - V(\mathbf{q})\chi(\mathbf{q},\omega), \tag{50}$$

which is also claimed to be exact. This is because χ is defined to be the response to the total potential

$$\rho^{ind}(\mathbf{q},\omega) = \chi|_{A\&M}(\mathbf{q},\omega)\phi(\mathbf{q},\omega) \tag{51}$$

which is very difficult to calculate since ϕ is self-consistently determined.

- The definitions of Fourier transforms

$$
\begin{aligned}
\chi(\mathbf{q},\omega) &= \int d^3(\mathbf{r}-\mathbf{r}')\int N(t-t')e^{i\mathbf{q}\cdot(\mathbf{r}-\mathbf{r}')}e^{-i\omega(t-t')}\chi(1,1') \\
c^\dagger_{\mathbf{k}}(t) &= \int d^3r e^{i\mathbf{k}\cdot\mathbf{r}}\hat{\psi}^\dagger(1) \\
c_{\mathbf{k}}(t) &= \int d^3r e^{-i\mathbf{k}\cdot\mathbf{r}}\hat{\psi}(1) \qquad (52)
\end{aligned}
$$

- the integral expression for the theta function

$$
\theta(t-t') = -\int \frac{d\omega'}{2\pi i}\,\frac{e^{-i\omega'(t-t')}}{\omega'+i\eta^+}, \qquad (53)
$$

where η^+ is a positive infinitesimal.[16]

- the solutions of the Heisenberg equation of motion $i\partial_t\hat{\mathcal{O}}_H(t) = [\hat{\mathcal{O}}_H(t),H]$ for $c^\dagger_{\mathbf{k}\sigma}(t)$ and $c_{\mathbf{k}\sigma}(t)$ for free fermions (check):

$$
c^\dagger_{\mathbf{k}\sigma}(t) = c^\dagger_{\mathbf{k}\sigma}e^{i\epsilon_{\mathbf{k}}t} \qquad (54)
$$

$$
c_{\mathbf{k}\sigma}(t) = c_{\mathbf{k}\sigma}e^{-i\epsilon_{\mathbf{k}}t} \qquad (55)
$$

- The commutator (check!)

$$
[c^\dagger_{k_1}c_{k_2}, c^\dagger_{k_3}c_{k_4}] = \delta_{k_2k_3}c^\dagger_{k_1}c_{k_4} - \delta_{k_1k_4}c^\dagger_{k_3}c_{k_2} \qquad (56)
$$

- The expectation values in the noninteracting ensemble of the number operator at finite temperature T are

$$
\langle\hat{n}_{\mathbf{k}}\rangle = f(\epsilon_{\mathbf{k}}), \qquad (57)
$$

where f is the Fermi function.

[16]The sign of the infinitesimal is important. It determines in which complex half-plane the contour can be completed to evaluate the integral by Cauchy's theorem. Check it!

Then (supressing spin indices)

$$
\begin{aligned}
&\langle [n_H(1), n_H[1'] \rangle = \mathrm{Tr}(\hat{\rho}_0 [n_H(1), n_H[1'])\\
= &\sum_{\mathbf{k}_1 \ldots \mathbf{k}_4} e^{i(\mathbf{k}_1-\mathbf{k}_2)\cdot \mathbf{r}} e^{i(\mathbf{k}_3-\mathbf{k}_4)\cdot \mathbf{r}'} \langle [c^\dagger_{\mathbf{k}_1}(t) c_{\mathbf{k}_2}(t), c^\dagger_{\mathbf{k}_3}(t') c_{\mathbf{k}_4}(t')] \rangle\\
= &\sum_{\mathbf{k}_1 \ldots \mathbf{k}_4} e^{i(\mathbf{k}_1-\mathbf{k}_2)\cdot \mathbf{r}} e^{i(\mathbf{k}_3-\mathbf{k}_4)\cdot \mathbf{r}'} e^{i([\epsilon_{\mathbf{k}_3}-\epsilon_{\mathbf{k}_4}]t' + [\epsilon_{\mathbf{k}_1}-\epsilon_{\mathbf{k}_2}]t)} \langle [c^\dagger_{\mathbf{k}_1} c_{\mathbf{k}_2}, c^\dagger_{\mathbf{k}_3} c_{\mathbf{k}_4}] \rangle\\
= &\sum_{\mathbf{k}_1 \mathbf{k}_2} e^{i(\mathbf{k}_4\cdot[\mathbf{r}-\mathbf{r}'] + \mathbf{k}_3\cdot[\mathbf{r}'-\mathbf{r}])} e^{i(\epsilon_{\mathbf{k}_3}-\epsilon_{\mathbf{k}_4})(t'-t)} \langle \hat{n}_{\mathbf{k}_3} \rangle\\
&\qquad - \sum_{\mathbf{k}_3 \mathbf{k}_4} e^{i(\mathbf{k}_4\cdot[\mathbf{r}-\mathbf{r}'] + \mathbf{k}_3\cdot[\mathbf{r}'-\mathbf{r}])} e^{i(\epsilon_{\mathbf{k}_3}-\epsilon_{\mathbf{k}_4})(t'-t)} \langle \hat{n}_{\mathbf{k}_4} \rangle
\end{aligned}
\tag{58}
$$

so that (using (46) and (52), and putting back the spin sum)

$$
\boxed{\chi_0(\mathbf{q}, \omega) = \sum_{\mathbf{k}\sigma} \frac{f(\xi_{\mathbf{k}}) - f(\xi_{\mathbf{k}+\mathbf{q}})}{\omega - (\xi_{\mathbf{k}+\mathbf{q}} - \xi_{\mathbf{k}}) + i\eta}}. \tag{59}
$$

This is the so-called Lindhard function, the charge susceptibility of the free Fermi gas. Note that in the free gas the major contributions to the integral (59) come from contributions where $\epsilon_{\mathbf{k}+q} - \epsilon_{\mathbf{k}} - \omega = 0$. These correspond to 2-particle "particle-hole excitations" where the Fermi sea is given a little energy ω which promotes a particle from below the Fermi surface (say $\mathbf{k}$) to above (say $\mathbf{k}+\mathbf{q}$). In the homework you will investigate when such excitations are possible within this model.

The use of the free gas susceptibility χ_0 for χ in Eq. (49) is a rather poor approximation, as it completely ignores the effect of the long-range Coulomb interaction on the intermediate states. The self-consistent field method, or random phase approximation, replaces the induced charge without interactions with the screened charge:

$$\chi_0 \equiv \left.\frac{\rho^{ind}}{\phi^{ext}}\right|_{V=0} \rightarrow \frac{\rho^{ind}|_{V=0}/\epsilon}{\phi^{ext}} = \frac{\chi_0}{\epsilon}. \qquad (60)$$

Solving (49) for ϵ gives

$$\boxed{\epsilon(\mathbf{q},\omega) \simeq 1 - V(\mathbf{q})\chi_0(\mathbf{q},\omega)} \qquad (RPA/SCF) \qquad (61)$$

This is sometimes called the Lindhard approx. to the dielectric function.

2.2.6 Thomas-Fermi theory

Let us consider the static limit of the theory we currently have. This will allow us to answer the original question we posed: if we insert a charge somewhere into a metal, what is the net electrostatic potential felt at some distance r away by a second charge? Taking the $\omega \rightarrow 0$ limit in (59), we find

$$\chi_0(\mathbf{q},0) = \sum_{\mathbf{k}\sigma} \frac{f(\varepsilon_{\mathbf{k+q}}) - f(\varepsilon_{\mathbf{k}})}{\varepsilon_{\mathbf{k}+q} - \varepsilon_k + i\eta^+} \qquad (62)$$

First note that if we further take the limit $q \rightarrow 0$ we find (recall N_0 is double-spin dos!)

$$\chi_0 \;\rightarrow\; -2\sum_k \frac{-\partial f}{\partial \varepsilon_{\mathbf{k}}} \simeq -N_0 \int d\xi_{\mathbf{k}}\, \frac{-\partial f}{\partial \xi_{\mathbf{k}}} \underbrace{\simeq}_{T \ll \epsilon_F} - N_0 \int d\xi_{\mathbf{k}} \delta(\xi_{\mathbf{k}}) = -N_0. \qquad (63)$$

The dielectric constant in the long-wavelength (i.e. small q) limit may thus be written

$$\epsilon(q,0) \simeq 1 + \frac{4\pi e^2}{q^2} N_0 \equiv 1 + \frac{k_{TF}^2}{q^2}, \tag{64}$$

where k_{TF} is the same Thomas-Fermi wave vector $k_{TF}^2 \equiv 4\pi e^2 N_0$ we discussed earlier. Now we go back: if we had placed a charge e in a vacuum, it would have produced a potential $\phi^{ext}(r) = e/r$, or $\phi^{ext}(q) = 4\pi e/q^2$ everywhere in space. From (41) we see that the actual potential in the medium is

$$\phi(q) = \phi^{ext}(q)/\epsilon(q) = \frac{4\pi e/q^2}{1 + k_{TF}^2/q^2} = \frac{4\pi e}{k_{TF}^2 + q^2}, \tag{65}$$

i.e. the Thomas-Fermi wavevector *cuts off* the divergence of the bare long-range Coulomb interaction. In real space

$$\boxed{\phi(\mathbf{r}) = \sum_{\mathbf{q}} e^{i\mathbf{q}\cdot\mathbf{r}} \phi(\mathbf{q}) = \frac{e}{r} e^{-k_{TF} r}}, \tag{66}$$

so the long-range interaction is indeed replaced by an exponentially cut off short-range one, with *screening length* scale k_{TF}^{-1}.

2.2.7 Friedel oscillations

The Thomas-Fermi theory is very intuitive and describes realistically how the singularities of the long-range Coulomb interaction are cut off by screening. It suffices to eliminate the anomalies encountered in Hartree-Fock theory of transport and density of states near the Fermi level. But because it is a long-wavelength approximation, it cannot describe adequately the response of the electron gas to a short-range perturbation. Our initial example of a point charge placed in an electron gas was just such a case. To get an accurate description of the screened impurity potential, the finite-q dependence of the charge susceptibility must be accounted for. This calculation involves simply replacing our Thomas-Fermi dielectric function $\varepsilon_{TF} = 1 - k_{TF}^2/q^2$ with the expression involving the full Lindhard function

$$\varepsilon_{Lindhard} = 1 - V(q)\chi_0(q,\omega=0) = 1 - \frac{k_{TF}^2}{q^2} F(\frac{q}{2k_F}), \qquad (67)$$

where F is the same function as in (19). Then we repeat the same calculation for the impurity potential

$$\phi(\mathbf{r}) \;=\; \sum_{\mathbf{q}} e^{i\mathbf{q}\cdot\mathbf{r}} \frac{\phi^{ext}(\mathbf{q})}{1 - \frac{k_{TF}^2}{q^2} F(\frac{q}{2k_F})} \simeq \frac{x^2}{(2+x^2)^2} \frac{\cos 2k_F r}{r^3}, \qquad (68)$$

where $x = k_{TF}/(2k_F)$. The main interesting feature of this result is of course the fact that the potential no longer has the simple Yukawa form with exponential decay, but in fact an *oscillatory* $1/r^3$ behavior. The last step in (68) is a bit long,[17] but I have attempted to give you a flavor of it in the homework. One of the main conclusions of the exercise there is that the potential is very sensitive to the details of the charge susceptibility at $2k_F$, which the Thomas-Fermi theory clearly

[17] See e.g. Fetter & Wallecka

gets wrong. Ultimately Friedel oscillations (and RKKY oscillations, their counterpart for magnetic spins) originate from the sharpness of the Fermi surface.

2.2.8 Plasmons

An examination of the dielectric function of the solid, e.g. Eq. (49), shows that the dielectric function can be zero, meaning the system responds very strongly to a small perturbation (see Eq. (41). These are the excitation energies of the electron gas. In the random phase approximation (61) this means there are excitations when

$$V(\mathbf{q})\chi_0(\mathbf{q},\omega) = 1 \tag{69}$$

Consider first a finite size box where the energy levels $\epsilon_{\mathbf{k}}$ are discrete. This means $\chi_0(\mathbf{q},\omega)$ is a sum of terms containing simple poles at the particle-hole excitation energies $\omega_{\mathbf{q}}(\mathbf{k}) \equiv \epsilon_{\mathbf{k}+\mathbf{q}} - \epsilon_{\mathbf{k}}$. χ_0 will change sign and diverge as ω passes through these energies, therefore there will be a solution of (69) for each excitation energy. It is simplest to focus on the limit at $T = 0$, where

$$\sum_{\substack{k<k_F \\ |\mathbf{k}+\mathbf{q}|>k_F}} \left\{ \frac{1}{\omega - (\xi_{\mathbf{k}+\mathbf{q}} - \xi_{\mathbf{k}}) + i\eta} - \frac{1}{\omega - (\xi_{\mathbf{k}} - \xi_{\mathbf{k}+\mathbf{q}}) + i\eta} \right\} \tag{70}$$

In other words, the poles in the complex ω plane are particle-hole excitation energies $\pm\omega_{\mathbf{k}}(\mathbf{q}) \equiv \xi_{\mathbf{k}+\mathbf{q}} - \xi_{\mathbf{k}}$, where $|\mathbf{k}+\mathbf{q}|$ is always above

Fermi surface and $\mathbf{k}$ always below.[18] The situation is depicted in figure 4. At $T=0$, there is a maximum frequency above which there are no

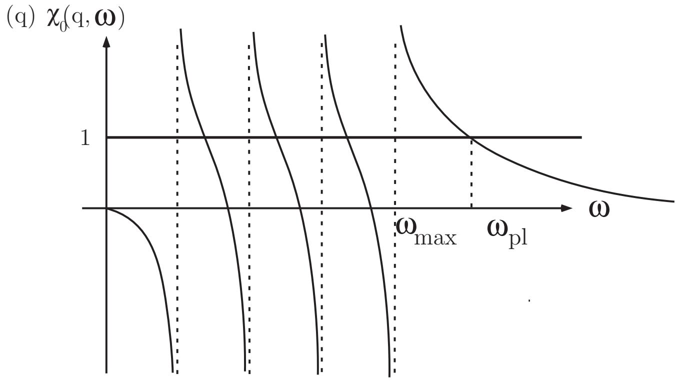


Figure 4: Eigenfrequencies of electron gas in RPA.

more particle-hole excitations possible for given fixed q, i.e. the largest excitation energy occurs when $k=k_F$ and $\mathbf{k},\mathbf{q}$ are parallel, so that for a parabolic band, $\epsilon_{\mathbf{k}}=k^2/(2m)$,

$$\omega_{max}=\frac{k_F q}{m}+\frac{q^2}{2m}. \tag{71}$$

[18]To arrive at this result, note from (59)

$$\begin{aligned}
\chi_0(\mathbf{q},\omega) &= \sum_{\mathbf{k}}\frac{f(\xi_{\mathbf{k}})-f(\xi_{\mathbf{k+q}})}{\omega-(\xi_{\mathbf{k+q}}-\xi_{\mathbf{k}})+i\eta}= \\
&= \sum_{\mathbf{k}}\frac{f(\xi_{\mathbf{k}})(1-f(\xi_{\mathbf{k+q}}))-f(\xi_{\mathbf{k+q}})(1-f(\xi_{\mathbf{k}}))}{\omega-(\xi_{\mathbf{k+q}}-\xi_{\mathbf{k}})+i\eta}= \\
&= \sum_{\mathbf{k}}\left\{\frac{f(\xi_{\mathbf{k}})(1-f(\xi_{\mathbf{k+q}}))}{\omega-(\xi_{\mathbf{k+q}}-\xi_{\mathbf{k}})+i\eta}-\frac{f(\xi_{\mathbf{k+q}})(1-f(\xi_{\mathbf{k}}))}{\omega-(\xi_{\mathbf{k+q}}-\xi_{\mathbf{k}})+i\eta}\right\} \\
&= \sum_{\mathbf{k}}\left\{\frac{f(\xi_{\mathbf{k}})(1-f(\xi_{\mathbf{k+q}}))}{\omega-(\xi_{\mathbf{k+q}}-\xi_{\mathbf{k}})+i\eta}-\frac{f(\xi_{\mathbf{k}})(1-f(\xi_{\mathbf{k-q}}))}{\omega-(\xi_{\mathbf{k}}-\xi_{\mathbf{k-q}})+i\eta}\right\} \\
&= \sum_{\mathbf{k}}\left\{\frac{f(\xi_{\mathbf{k}})(1-f(\xi_{\mathbf{k+q}}))}{\omega-(\xi_{\mathbf{k+q}}-\xi_{\mathbf{k}})+i\eta}-\frac{f(\xi_{-\mathbf{k}})(1-f(\xi_{-\mathbf{k}-\mathbf{q}}))}{\omega-(\xi_{-\mathbf{k}}-\xi_{-\mathbf{k}-\mathbf{q}})+i\eta}\right\} \\
&= \sum_{\mathbf{k}}\left\{\frac{f(\xi_{\mathbf{k}})(1-f(\xi_{\mathbf{k+q}}))}{\omega-(\xi_{\mathbf{k+q}}-\xi_{\mathbf{k}})+i\eta}-\frac{f(\xi_{\mathbf{k}})(1-f(\xi_{\mathbf{k+q}}))}{\omega-(\xi_{\mathbf{k}}-\xi_{\mathbf{k+q}})+i\eta}\right\} \\
&= \sum_{\mathbf{k}}f(\xi_{\mathbf{k}})(1-f(\xi_{\mathbf{k+q}}))\left\{\frac{1}{\omega-(\xi_{\mathbf{k+q}}-\xi_{\mathbf{k}})+i\eta}-\frac{1}{\omega-(\xi_{\mathbf{k}}-\xi_{\mathbf{k+q}})+i\eta}\right\} \\
\lim_{T\to 0} &= \sum_{\substack{k<k_F\\ |\mathbf{k+q}|>k_F}}\left\{\frac{1}{\omega-(\xi_{\mathbf{k+q}}-\xi_{\mathbf{k}})+i\eta}-\frac{1}{\omega-(\xi_{\mathbf{k}}-\xi_{\mathbf{k+q}})+i\eta}\right\}
\end{aligned}$$

There is another possible root of ϵ, as also shown in Fig. (4). In the limit $\omega > \omega_{max}$, we may expand (70) for small q, and find

$$\begin{aligned}
\chi(\mathbf{q},\omega) &\simeq -\frac{2q^2}{m\omega^2}\sum_{k<k_F}\left[1+\frac{2\mathbf{k}\cdot\mathbf{q}}{m\omega}+3\left(\frac{\mathbf{k}\cdot\mathbf{q}}{m\omega}\right)^2+\ldots\right] \\
&\simeq -\frac{k_F^3}{3\pi^2}\frac{q^2}{m\omega^2}\left[1+\frac{3}{5}\left(\frac{k_F q}{m\omega}\right)^2+\ldots\right]. \qquad (72)
\end{aligned}$$

Now we look for a solution to $\mathrm{Re}V\chi_0 = 1$ and find to leading order[19]

$$\omega = \omega_{pl}\left(1+\mathcal{O}(q/k_F)^2+\ldots\right), \qquad (73)$$

with

$$\omega_{pl} = \left(\frac{4\pi n e^2}{m}\right)^{1/2} \qquad (74)$$

which is of course the plasma frequency you found by elementary methods last semester. In contrast to the particle-hole excitations, which involve exciting only 1 particle from its position in the Fermi sea, a plasma oscillation perforce involves motions of all particles and is therefore referred to as a collective mode of the system. Plasmons have been observed indirectly in metals, primarily in thin metallic films.

2.3 Fermi liquid theory

In a good metal the average interelectron distance is of the order of or smaller than the range of the interaction, e.g. the screening length

[19] Note this is a result for 3 dimensions. It is a useful exercise to obtain the analagous result for 2D, which has $\omega \sim q^{1/2}$, i.e a gapless mode.

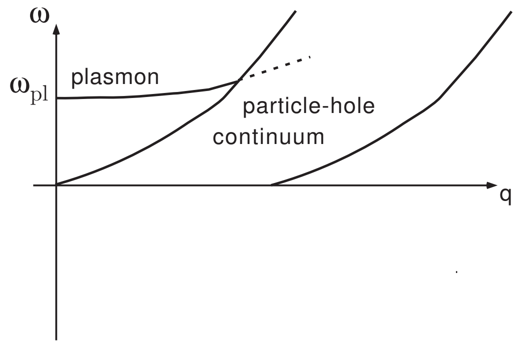


Figure 5: Excitations (poles of $\epsilon(\mathbf{q},\omega)^{-1}$) at $T=0$.

$k_{TF}^{-1} \approx 0.5\left(n/a_0^3\right)^{-1/6}$, where n is the density, of order 0.1-1nm for typical parameters. One might therefore expect that interactions should strongly modify the picture of free electrons commonly used to describe metals. It turns out, however, that for $T \ll T_F$ the important degrees of freedom are mostly frozen out, and only a fraction T/T_F of all electrons near the Fermi surface participate in interaction processes. This leads to the possibility of a mapping between the free Fermi gas and the interacting Fermi system. IF the elementary excitations of the many-body system can be obtained from the single-particle states of the free electron gas by turning on the interaction adiabatically (and if the ground state has the full symmetry of the Hamiltonian), the distribution function $n_{k\sigma}$ of the interacting system would be the same as that of a free gas, and the particle and hole excitations of the gas would evolve into "quasiparticle" and "quasihole" states.

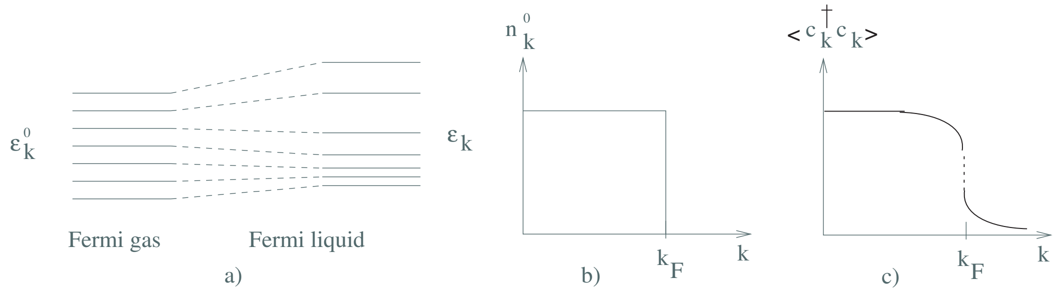


Figure 6: a) Evolution of quasiparticle states; b) $T = 0$ Quasiparticle distribution function n^0_k; c) $T = 0$ true electron distribution function $\langle c^\dagger_{\mathbf{k}} c_{\mathbf{k}} \rangle$.

2.3.1 Particles and holes

To understand what this really means, let's go back and review the definitions of the terms particles and holes. Let's take N free Fermions, mass m in a volume L^3, where we know that the eigenstates are Slater determinants of N different single particle states, each given by

$$\psi_{\mathbf{k}}(\mathbf{r}) = \frac{1}{\sqrt{L^3}} e^{i\mathbf{k}\cdot\mathbf{r}}. \tag{75}$$

Let's stick to $T = 0$ for the moment, and recall that the occupation of each state is given by $n_{\mathbf{k}} = \theta(k - k_F)$, where k_F is the radius ermi sea.

Now let's add one "test" particle to the lowest available state $k = k_F$. We then have for the chemical potential at $T = 0$,

$$\mu = E_0(N+1) - E_0(N) = \frac{\partial E_0}{\partial N} = \frac{k_F^2}{2m}. \tag{76}$$

Particles and holes are excitations of the filled Fermi sea. Excitations of the gas consist of taking a certain number of particles and moving them to the other side of the Fermi surface, yielding particles above and an equal number of holes below the Fermi surface. These excitations can be described in terms of the changes in the particle occupation numbers $\delta n_p = n_p - n_p^0$:

$$\delta n_k = \begin{cases} \delta_{k,k'} \text{ for a particle } k' > k_F \\ -\delta_{k,k'} \text{ for a hole } k' < k_F \end{cases} . \tag{77}$$

At nonzero temperatures, a thermal fluctuation will create changes in

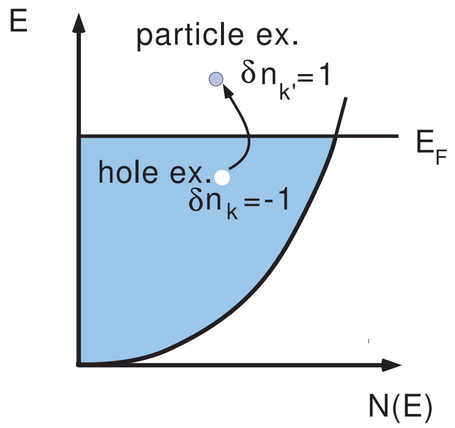


Figure 7: *Particle and hole excitations of the Fermi gas.*

occupation numbers $\delta n_p \sim 1$ only for excitations of energy within $k_B T$ of ε_F. Note that the total energy of the free gas is completely specified as a functional of the occupation numbers:

$$E - E_0 = \sum_{\mathbf{k}} \frac{k^2}{2m}(n_k - n_k^0) = \sum_{\mathbf{k}} \frac{k^2}{2m} \delta n_k . \tag{78}$$

Now take the gas and put it in contact with a particle reservoir. The appropriate thermodynamic potential is then the Gibbs free energy, which for $T = 0$ is $F = E - \mu N$, and

$$F - F_0 = \sum_{\mathbf{k}} \left(\frac{k^2}{2m} - \mu \right) \delta n_k \equiv \sum_k \xi_k \delta n_k \, . \tag{79}$$

The free energy of one particle, with momentum $\mathbf{k}$ and occupation $\delta n_{\mathbf{k}'} = \delta_{\mathbf{k},\mathbf{k}'}$ is $\xi_{\mathbf{k}}$ and it corresponds to an excitation outside the Fermi surface. The free energy of a hole $\delta n_{\mathbf{k}'} = -\delta_{\mathbf{k},\mathbf{k}'}$ is $-\xi_{\mathbf{k}}$, which corresponds to an excitation below the Fermi surface. For both species then the free energy of an excitation is $|\xi_k|$, which is always positive; ie., the Fermi gas is stable with respect to excitations as it must be.
Quasiparticles and quasiholes in interacting system

Consider a system with interacting particles an average spacing a apart, so that the typical interaction energy is $\frac{e^2}{a} e^{-a/r_{TF}}$. As discussed above, we now suppose that we can create this system by turning on the interactions adiabatically starting from the free gas in a time t, such that the system evolves while staying always in its ground state.

If a state of the ideal system is characterized by the distribution $n^0_{\mathbf{k}}$, then the state of the interacting system will evolve adiabatically from $n^0_{\mathbf{k}}$ to $n_{\mathbf{k}}$. In fact if the system remains in its ground state, then $n^0_{\mathbf{k}} = n_{\mathbf{k}}$, i.e. the occupation of each state labelled by $\mathbf{k}$ won't change (although the energy will). This is an assumption, and we will be studying some counterexamples to this ansatz (superconductivity and magnetism). But in general Landau expected this to hold if the *symmetry* of the interacting system was the same as the noninteracting one, and this appears to be the case for simple metals.

Let's follow what happens to a particle of momentum $\mathbf{k}$ added to the top of the non-interacting Fermi gas when we slowly turn the interaction knob. As U increases, two things happen. The $\mathbf{k}$ state of the

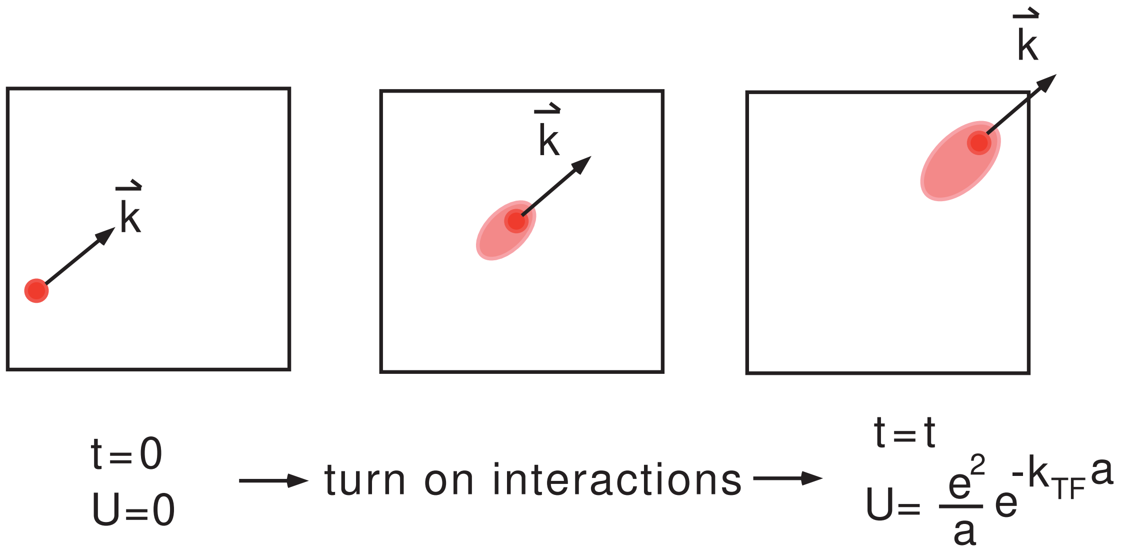


Figure 8: *Evolution of particle in state* $\mathbf{k}$ *on top of Fermi sea as interaction is turned on. Particle becomes "dressed" by interactions with the rest of the system which changes the effective mass but not the momentum of the excitation ("quasiparticle").*

original particle is no longer an eigenstate of $\mathcal{H}$, so it decays into the new excitations of the system, which according to our ansatz are also single-particle-like. Nearby particles also decay into the original state; this mixing has the effect of "dressing" the original free particle with a "cloud" of excitations of the surrounding system. However since momentum is conserved, the net excitation (called a *quasiparticle*)) can still be labelled with original momentum $\mathbf{k}$. In the same way, holes of momentum **k** below the Fermi surface evolve into quasiholes. Occasionally an analogy from classical mechanics is useful: we think of a bullet being fired into a large container filled with cotton. It will drag some cotton with it, and create a "particle+cloud" with increased mass but the same momentum.

It is too much to hope that the interactions between quasiparticles will vanish altogether. The N-particle ground state wave-function may still be Slater-determinant like, but this doesn't necessarily imply that the quasiparticles are infinitely long-lived (exact) eigenstates of the system. So if each quasiparticle state **k** has lifetime $\tau_{\mathbf{k}}$, we have to worry a bit about the adiabatic switching on procedure if $\tau_{\mathbf{k}} < t$. If so, the quasiparticle will decay before we finish switching, and we won't be able to go reversibly back and forth. If we decrease t too much so again $\tau_{\mathbf{k}} \gg t$, then the switching on of U may not be adiabatic, i.e. we may knock the system into a state other than its ground state. It was Landau's great insight to recognize that these objections are overcome for quasiparticle states sufficiently close to the Fermi energy. In this case the Pauli principle strongly restricts the decay channels for a quasiparticle, and one can argue (see below) that the lifetime becomes infinite at the Fermi energy itself. Therefore for any time t there should be a narrow range of energies near the Fermi surface for which the $\tau_{\mathbf{k}}$ is long enough to make the whole construction work.

2.3.2 Energy of quasiparticles.

As in the free gas, excitations will be characterized only by the deviation of the occupation number from the ground state occupation $n^0_{\mathbf{k}}$.[20]

$$\delta n_{\mathbf{k}} = n_{\mathbf{k}} - n^0_{\mathbf{k}} \,. \tag{80}$$

At suffiently low temperatures $\delta n_{\mathbf{k}} \sim 1$ only for those excitations near the Fermi surface where the condition $\tau_{\mathbf{k}} \gg t$ is satisfied. Therefore we should be able to formulate a theory which depends only on $\delta n_{\mathbf{k}}$, not on $n_{\mathbf{k}}$ or $n^0_{\mathbf{k}}$, which are not well defined for $\mathbf{k}$ far from the Fermi surface. $n_{\mathbf{k}}$ and $n^0_{\mathbf{k}}$ should never enter independently and are not physically relevant.

For the noninteracting system the dependence of the energy ($T = 0$) E on $\delta n_{\mathbf{k}}$ is very simple:

$$E - E_0 = \sum_{\mathbf{k}} \frac{k^2}{2m} \delta n_{\mathbf{k}} \,. \tag{81}$$

In the interacting case $E[n_{\mathbf{k}}]$ is more complicated generally, but if we take $\delta n_{\mathbf{k}}$ to be small (just a few excitations above the ground state) then we may expand:

$$E[n_{\mathbf{k}}] = E_o + \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} \delta n_{\mathbf{k}} + \mathcal{O}(\delta n^2_{\mathbf{k}}) \,, \tag{82}$$

[20] Note we will now take over the notation $n^0_{\mathbf{k}}$ which in the previous discussion meant the distribution function of the noninteracting system. Now it means the ground state of the interacting system. They are the same by Landau's ansatz.

where we now *define* $\epsilon_{\mathbf{k}} = \delta E/\delta n_{\mathbf{k}}$. If $\delta n_{\mathbf{k}} = \delta_{\mathbf{k},\mathbf{k}'}$, then $E \approx E_0 + \epsilon_{\mathbf{k}'}$; i.e., the energy of the quasiparticle with momentum $\mathbf{k}'$ is $\epsilon_{\mathbf{k}'}$.

As discussed, we will only need $\epsilon_{\mathbf{k}}$ near the Fermi surface where $\delta n_{\mathbf{k}}$ is $\mathcal{O}(1)$. So we may expand $\epsilon_{\mathbf{k}}$ around the Fermi level,

$$\epsilon_{\mathbf{k}} \approx \mu + (\mathbf{k} - \mathbf{k}_F) \cdot \nabla_k \, \epsilon_{\mathbf{k}}|_{k_F} \tag{83}$$

where $\nabla_k \epsilon_{\mathbf{k}} = v_{\mathbf{k}}$, the group velocity of the quasiparticle. We no longer know the exact form of $\epsilon_{\mathbf{k}}$, but some exact relations must be obeyed because our system obeys certain symmetries. If we explicitly put the spin-dependence back in, we have symmetries

$$\epsilon_{\mathbf{k},\sigma} = \epsilon_{-\mathbf{k},-\sigma} \quad \text{time-reversal} \tag{84}$$

$$\epsilon_{\mathbf{k},\sigma} = \epsilon_{-\mathbf{k},\sigma} \quad \text{parity} \tag{85}$$

So unless we explicitly break T-symmetry by e.g. applying a magnetic field, we have $\epsilon_{\mathbf{k},\sigma} = \epsilon_{-\mathbf{k},\sigma} = \epsilon_{\mathbf{k},-\sigma}$. Furthermore, as usual $\epsilon_{\mathbf{k}}$ has to respect the point and space group symmetries of the system, e.g. for an isotropic system $\epsilon_{\mathbf{k}}$ depends only upon the magnitude of $\mathbf{k}$, $|\mathbf{k}|$, so $\mathbf{k}$ and $v_{\mathbf{k}} = \nabla \epsilon_{\mathbf{k}}(|\mathbf{k}|) = \hat{k}(d\epsilon_k/dk)$ are parallel.[21] Define $(m^*)^{-1}$ as the constant of proportionality at the Fermi surface[22]

$$v_{k_F} = k_F/m^* \tag{86}$$

[21] For a cubic system $\epsilon_{\mathbf{k}}$ is invariant under $90°$ rotations, etc.

[22] Note k_F is not changed by interactions (Luttinger's theorem for isotropic system)

Then for the interacting system at the Fermi surface

$$N_{interacting}(\varepsilon_F) = \frac{m^* k_F}{\pi^3}\,, \tag{87}$$

the same *form* as for the noninteracting system. Note the m^* (usually but not always $> m$) accounts for the dressing of the quasiparticle particle (bullet + cotton!). In other words, as far as the density of levels at the Fermi energy is concerned, the only thing which changes is the effective mass of the fermionic single-particle excitations.

2.3.3 Residual quasiparticle interactions

Let's go back to the Gibbs free energy of our system of quasiparticles characterized in some generalized excited state by distribution function $\delta n_{\mathbf{k}}$:

$$F - F_0 = E - E_0 - \mu(N - N_0)\,. \tag{88}$$

where again F_0, E_0 etc. characterize the ground state. Thus,

$$N - N_0 = \sum_{\mathbf{p}} \delta n_{\mathbf{k}}\,, \tag{89}$$

and since

$$E - E_0 \approx \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} \delta n_{\mathbf{k}} + \mathcal{O}(\delta n^2)\,, \tag{90}$$

we get

$$F - F_0 \approx \sum_{\mathbf{k}} (\epsilon_{\mathbf{k}} - \mu)\, \delta n_{\mathbf{k}} = \sum_{\mathbf{k}} \xi_{\mathbf{k}} \delta n_{\mathbf{k}} + \mathcal{O}(\delta n^2)\,. \tag{91}$$

As shown in Fig. 9, we will be interested in excitations of the system which deform the Fermi surface by an amount proportional to δ. For example, along the positive k_x axis, our excited system has $\delta n_{\mathbf{k}} = 1$ for some states $\mathbf{k}$ above k_F, whereas along the negative k_x axis some states have $\delta n_{\mathbf{k}} = -1$. The approximation to the free energy above will

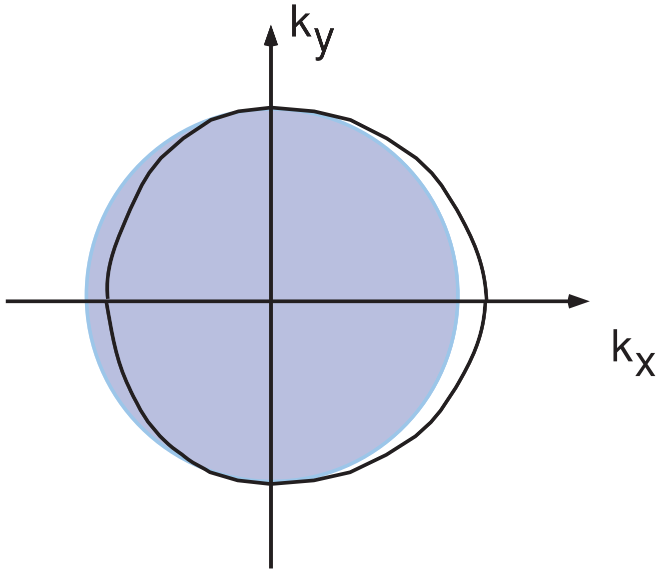


Figure 9: *Small deformations of the Fermi sphere, proportional to δ.*

remain valid provided

$$\frac{1}{N}\sum_{\mathbf{k}} |\delta n_{\mathbf{k}}| \ll 1 \,. \tag{92}$$

If we stick with our original criterion of using only states near the Fermi surface to construct our distortion, the $\xi_{\mathbf{k}}$ for those states with $\delta n_{\mathbf{k}} \neq 0$ will also be of order δ. Thus,

$$\sum_{\mathbf{k}} \xi_{\mathbf{k}} \delta n_{\mathbf{k}} \sim \mathcal{O}(\delta^2)\,, \tag{93}$$

so in order to keep terms of order δ^2 consistently we must also add the next term in the Taylor series expansion of the energy :

$$\boxed{F - F_0 = \sum_{\mathbf{k}} \xi_{\mathbf{k}} \delta n_{\mathbf{k}} + \frac{1}{2} \sum_{\mathbf{k},\mathbf{k}'} f_{\mathbf{k},\mathbf{k}'} \delta n_{\mathbf{k}} \delta n_{\mathbf{k}'} + \mathcal{O}(\delta^3)} \tag{94}$$

where

$$f_{\mathbf{k},\mathbf{k}'} = \frac{\delta E}{\delta n_{\mathbf{k}} \delta n_{\mathbf{k}'}} \tag{95}$$

The term proportional to $f_{\mathbf{k},\mathbf{k}'}$, was proposed by L.D. Landau. It describes the residual interactions of the quasiparticle excitations which remain even after they are "dressed". A glance at the dimensions of the new term shows that $f_{\mathbf{k},\mathbf{k}'} \sim 1/V$. But if $f_{\mathbf{k},\mathbf{k}'}$ is an interaction between quasiparticles, each of which (in plane-wave like state) is delocalized over the whole volume V, so the probability that two will interact is roughly $\sim k_{TF}^{-3}/V$. Therefore

$$\boxed{f_{\mathbf{k},\mathbf{k}'} \sim k_{TF}^{-3}/V} \tag{96}$$

We can proceed as earlier with the quasiparticle energy $\epsilon_{\mathbf{k}}$ and ask how this unknown interaction function reflects the underlying symmetries of the physical system. To this end we reintroduce the hidden spin degrees of freedom. First in the absence of an external magnetic field, the system should be invariant under time-reversal, so

$$f_{\mathbf{k}\sigma,\mathbf{k}'\sigma'} = f_{-\mathbf{k}-\sigma,-\mathbf{k}'-\sigma'} \ , \tag{97}$$

and, in a system with reflection symmetry (parity)

$$f_{\mathbf{k}\sigma,\mathbf{k}'\sigma'} = f_{-\mathbf{k}\sigma,-\mathbf{k}'\sigma'} \,. \tag{98}$$

Then since this implies

$$f_{\mathbf{k}\sigma,\mathbf{k}'\sigma'} = f_{\mathbf{k}-\sigma,\mathbf{k}'-\sigma'} \,. \tag{99}$$

it must be that f depends only upon the relative orientations of the spins σ and σ', so there are only two independent components for given $\mathbf{k}, \mathbf{k}'$, e.g. $f_{\mathbf{k}\uparrow,\mathbf{k}'\uparrow}$ and $f_{\mathbf{k}\uparrow,\mathbf{k}'\downarrow}$. It is more conventional to decompose f into spin-symmetric and antisymmetric parts:

$$f^a_{\mathbf{k},\mathbf{k}'} = \frac{1}{2}\left(f_{\mathbf{k}\uparrow,\mathbf{k}'\uparrow} - f_{\mathbf{k}\uparrow,\mathbf{k}'\downarrow}\right) \qquad f^s_{\mathbf{k},\mathbf{k}'} = \frac{1}{2}\left(f_{\mathbf{k}\uparrow,\mathbf{k}'\uparrow} + f_{\mathbf{k}\uparrow,\mathbf{k}'\downarrow}\right) \,. \tag{100}$$

$f^a_{\mathbf{k},\mathbf{k}'}$ may be interpreted as an exchange interaction, or

$$f_{\mathbf{k}\sigma,\mathbf{k}'\sigma'} = f^s_{\mathbf{k},\mathbf{k}'} + \boldsymbol{\sigma}\cdot\boldsymbol{\sigma}' f^a_{\mathbf{k},\mathbf{k}'} \tag{101}$$

where $\boldsymbol{\sigma}$ and $\boldsymbol{\sigma}'$ are the Pauli matrices for the spins.

The next important assumption entering Fermi liquid theory is that the quasiparticle interactions are short-ranged. This means that $f_{kk'}$ is essentially constant as a function of $|\vec{k}|, |\vec{k}'|$, and so depends only on the directions $\hat{k}, \hat{k}'$, $f^{s,a}_{kk'} \simeq f(\hat{k}, \hat{k}')$:

$$f_{\mathbf{k},\mathbf{k}'} \simeq f_{\mathbf{k},\mathbf{k}'}\big|_{\epsilon_{\mathbf{k}}=\epsilon_{\mathbf{k}'}=\mu} \tag{102}$$

or equivalently, only on the angle θ between them!

$$f^{\alpha}_{\mathbf{k},\mathbf{k}'} = \sum_{l=0}^{\infty} f^{\alpha}_{l} P_l(\cos\theta)\,. \tag{103}$$

Conventionally these f parameters are expressed in terms of dimensionless quantities.

$$VN_0 f^{\alpha}_{l} = \frac{Vm^* k_F}{\pi^2 \hbar^3} f^{\alpha}_{l} = F^{\alpha}_{l}\,. \tag{104}$$

We expect that the *Landau parameters* $F^{s,a}_{\ell}$ will be negligible for sufficiently large ℓ, so we have now achieved our goal of subsuming the complicated effects of interactions in a few phenomenological parameters.

2.3.4 Local energy of a quasiparticle

Now consider an interacting system with a certain distribution of excited quasiparticles $\delta n_{\mathbf{k}'}$. Let's add another particle, say of momentum $\mathbf{k}$ and see how the energy changes. The distribution function goes from $(\delta n'_{\mathbf{k}} \rightarrow \delta n'_{\mathbf{k}} + \delta_{\mathbf{k},\mathbf{k}'})$. From Eq. 94 the free energy of the additional quasiparticle is

$$\tilde{\xi}_k = \xi_{\mathbf{k}} + \sum_{\mathbf{k}'} f_{\mathbf{k}',\mathbf{k}} \delta n_{\mathbf{k}'}\,, \tag{105}$$

(since $f_{\mathbf{k}',\mathbf{k}} = f_{\mathbf{k},\mathbf{k}'}$). The second term on the right corresponds to the average interaction of a quasiparticle with the other quasiparticles in the system.[23]

Substituting (103) and (104) in (105) gives the shift in energy of a quasiparticle due to the Landau interaction

$$\delta\xi_{\mathbf{k}\sigma} \equiv \tilde{\xi}_k - \xi_{\mathbf{k}} = \frac{1}{N_0}[F_0^s\delta n + \sigma F_0^a \delta n_s + \frac{1}{k_F^2} F_1^s \vec{k}\cdot\vec{g} + ...], \tag{106}$$

where $\delta n = \Sigma_{k\sigma}\,\delta n_{k\sigma}$ is the density shift, $\delta n_s = \Sigma_{k\sigma}\,\sigma\delta n_{k\sigma}$ is the spin density shift, and $\vec{g} = \Sigma_{k\sigma}\,\vec{k}\delta n_{k\sigma}$ is the number current. The first two terms can be thought of as molecular field couplings representing the average effect of density and magnetization fluctuations in the surrounding medium on the quasiparticle energy. The third term is the famous "backflow" term which describes the effect of the quasiparticle streaming through the medium to which it couples. The flow pattern is of dipolar form, as depicted in Figure 10. Note that the Landau parameter F_1^s is not completely independent, as it can be shown that in a Galilean invariant system it is directly related to the effective mass by the relation $m^*/m = 1 + F_1^s/3$ (see below). In a crystal this relation does not hold.[24]

Before leaving this section, let me just mention that the importance of the *local quasiparticle energy* $\tilde{\xi}$ or rather the energy *shift* $\delta\tilde{\xi}$ is

[23]The structure may remind you of Hartree-Fock theory, to which it is similar, but keep in mind f is the residual interaction between quasiparticles, not electrons

[24]For an extensive discussion of this and many other aspects of FL theory I've glossed over, see G. Baym and C. Pethick, Landau Fermi-Liquid Theory : Concepts and Applications, Wiley 1991

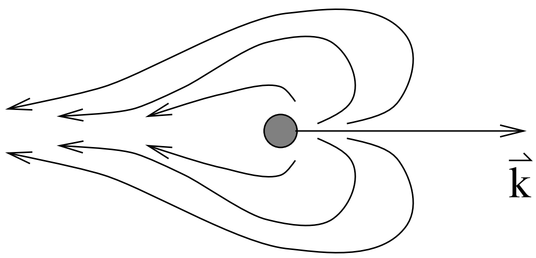


Figure 10: Schematic of backflow around quasiparticle of momentum $\mathbf{k}$

that when one writes down how external forces couple to the system to determine, e.g. transport properties, it is the gradient of $\tilde{\xi}_{\mathbf{k}}$ which is the force a qp of momentum $\mathbf{k}$ experiences due to spatial inhomogeneities in the system. There is a "Landau molecular field" proportional to

$$-\nabla\tilde{\delta}\xi_{\mathbf{k}} = -\nabla\sum_{\mathbf{k}'} f_{k'k}\delta n_{\mathbf{k}'}(\mathbf{r}) \tag{107}$$

which is responsible, e.g. for spin waves in dilute gases. Eq. (107) is a simplified version of Landau's famous kinetic equation for a Fermi liquid which is the analog of the Boltzman equation for a weakly interacting gas.

2.3.5 Thermodynamic properties

The expression (106) for the quasiparticle energies and the fact that the equilibrium quasiparticle distribution function is just the Fermi function enables immediate calculations of thermodynamic observables in the Fermi liquid. Because the states of the gas and liquid are in one to one correspondence, for example, one immediately knows that the expression for the entropy of the liquid is the same as that for a free Fermi gas,[25]

$$S = -\sum_{k\sigma}[n_{k\sigma}\log n_{k\sigma} + (1-n_{k\sigma})\log(1-n_{k\sigma})]. \tag{108}$$

Note now that the distribution function $n_{k\sigma}$ in *local equilibrium* must be a Fermi function evaluated at energy $\epsilon_{k\sigma}$ given by the bare energy plus the expression (105) in general. However, we are interested in calculating a quantity in *global equilibrium*, in which case the shifts $\delta n, \delta n_s, \vec{g}, ...$ vanish. In this case the calculation reduces to the usual one for a free Fermi gas. For temperatures $T \ll T_F$ we replace the sum $\Sigma_{k\sigma}$ by $N_0 \int d\xi$. The temperature can then be scaled out, and the remaining integral performed, yielding the entropy density at low temperatures,

$$s = \frac{1}{3}\pi^2 N_0 T, \tag{109}$$

and the specific heat at constant volume is therefore $C = T(\partial s/\partial T)_V = (m^* k_F/3)T$, where in the last step we have used $N_0 = m^* k_F/\pi^2$. The result for the liquid is identical to that for the gas, with the exception of the replacement of m by m^*.

Similarly, we may derive an expression for the spin susceptibility of the Fermi liquid by constructing the magnetization δn_s as above, and noting that the shift in the distribution function is due to the Landau

[25]Recall the *form* of the Fermi distribution function for the free gas is obtained purely from combinatorial considerations, not from any knowledge of the energies.

shift in the quasiparticle energy (molecular field) as well as the external field $\vec{H}$:

$$\delta n_{k\sigma} = \frac{\partial n_{k\sigma}}{\partial \epsilon_{k\sigma}}(\delta\epsilon_{k\sigma} - \mu_0 \sigma H). \tag{110}$$

Using $\delta n_s \equiv \Sigma_{k\sigma}\, \sigma\delta n_{k\sigma}$, and noting that since $\sigma\partial n/\partial\epsilon$ is isotropic and odd in σ, only the $\ell = 0$, spin-antisymmetric part of $\delta\epsilon_{k\sigma}$ contributes to the sum, we find for the spin susceptibility $\chi_0 = \mu_0(\partial n_s/\partial H)$

$$\chi = \frac{\mu_0^2 N_0}{(1+F_0^a)} = \frac{m^*/m}{1+F_0^a}\chi_0, \tag{111}$$

where χ_0 is the susceptibility of the free gas.

2.3.6 Quasiparticle relaxation time and transport properties.

Calculations of transport properties require introducing the quasiparticle lifetime. Recall the quasiparticle states are *not* eigenstates of the many-body Hamiltonian, due to the weak residual interactions among them. We therefore expect a quasiparticle with momentum $\vec{k}$ to decay except when it sits exactly at the Fermi surface and when $T = 0$, when it can easily be seen there is no phase space for scattering which conserves energy and momentum. But relaxing these conditions ($\vec{k}$ not on FS, $T \neq 0$) allows phase space for scattering and hence a finite lifetime.

Since the interactions among quasiparticles are assumed weak, we may use a golden rule type formula for the scattering rate"

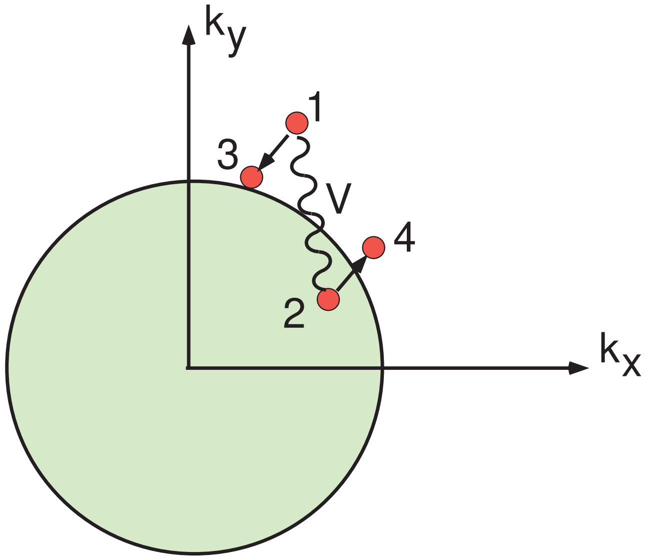


Figure 11: 2-quasiparticle collision: states before (1,2) and after (3,4)

Let's consider a quasiparticle with energy $\xi_1 = \epsilon_1 - \mu$ above the Fermi level. A scattering process takes it to final state ξ_3, and to conserve energy and momentum a quasiparticle with energy ξ_2 must be scattered to final state ξ_4. I've assumed the interaction V is independent of momentum, frequency, etc. because the most important effects we are looking for are purely statistical, unless V is very singular.[26] The "golden rule" then gives

$$\begin{aligned}\frac{1}{\tau_1} &= 2\pi \int d\xi_2 N(\xi_2) \int d\xi_3 N(\xi_3) \int d\xi_4 N(\xi_4) |V|^2 f(\xi_2)(1-f(\xi_3))(1-f(\xi_4))\delta(\xi_1+\xi_2-\xi_3-\xi_4) \simeq \\ &\simeq 2\pi N_0^3 |V^2| \int_0^{\xi_1} d\xi_3 \int_0^{\xi_1-\xi_3} d\xi_4 = \pi N_0^3 |V|^2 \xi_1^2,\end{aligned}$$

[26]In the case of the Coulomb interaction, which is very singular, screening takes care of this problem. See section 2.2.6

where the delta function conserves energy and the Fermi factors ensure that there is a particle in state 2 and that states 3 and 4 are empty beforehand. For simplicity I evaluated the Fermi functions at T=0, giving the final simple result. Note I have neglected spin for the moment, but this is not essential.[27] Note now that for $N_0 V \ll 1$ (weak residual interactions) and $N_0 \sim 1/\varepsilon_F$, it is clear that for $\xi \ll \varepsilon_F$ the scattering satisfies the condition

$$\frac{1}{\tau_1} \ll \xi. \tag{112}$$

This means that the quasiparticle states are well-defined near the Fermi surface, since their damping is small compared to the energy of the state. (As expected, the relaxation rate exactly at the Fermi surface vanishes identically.) We therefore expect that Fermi liquid theory calculations in terms of a weakly interacting quasiparticle gas will be valid for frequencies and temperatures such that $\omega, T \ll \varepsilon_F$.

Two further comments about the scattering rate are of potential importance. First, I give without proof the full result at finite tempera-

[27] What I have done which is not really Kosher, however, is to neglect the constraints placed on the scattering by momentum conservation. It turns out in three dimensions this is not terribly important, and one obtains the correct answer. It is a useful exercise to convince yourself, for example, that in 2D the relaxation rate goes like $\xi^2 \log \xi$.

tures:[28]

$$\frac{1}{\tau(\xi)} = \frac{\pi|V|^2}{64\varepsilon_F^3}[(\pi T)^2 + \xi^2], \tag{114}$$

so that at finite T one finds that $1/\tau$ varies as T^2 or ξ^2, whichever is larger. Certain simple transport properties in a Fermi liquid reflect this directly. For example, the resistivity due to electron-electron scattering in a metal goes as T^2 at the lowest temperatures; it is usually masked by other, larger sources of scattering in ordinary metals, however.[29] The second remark is that if one were to find, for some microscopic model, that the relaxation rate was larger than the quasiparticle energy, the quasiparticles would be overdamped and the entire concept would be useless. One would then speak of an incoherent or "non-Fermi liquid"

---

[28] Our simple calculation has to be modified to account for momentum conservation, expressed as

$$\mathbf{k}_1 - \mathbf{k}_3 = \mathbf{k}_4 - \mathbf{k}_2 \,. \tag{113}$$

Since ξ_1 and ξ_2 are confined to a narrow shell around the Fermi surface, so too are ξ_3 and ξ_4. This can be seen in Fig. 11, where the requirement that $\mathbf{k}_1 - \mathbf{k}_3 = \mathbf{k}_4 - \mathbf{k}_2$ limits the allowed states for particles 3 and 4. Taking $\mathbf{k}_1$ fixed, allowed momenta for 2 and 3 are obtained by rotating $\mathbf{k}_1 - \mathbf{k}_3 = \mathbf{k}_4 - \mathbf{k}_2$; this rotation is constrained, however, by the fact that particles cannot scatter into occupied states. This restriction on the final states reduces the scattering probability by a factor of ξ_1/ε_F, but is the same restriction contained in the calculation above. Thus momentum conservation doesn't affect our $T = 0$ estimate above, except to modify the prefactor.

If these hand-waving arguments don't satisfy you (they shouldn't), see AGD or Fetter/Wallecka.

[29] Of course this is not quite right. The electron-electron interactions in a solid conserve crysal momentum, and thus the conductivity of a pure crystal would be infinite at any temperature unless one explicitly accounts for Umklapp processes. Thus it is *not* true for the electrical conductivity that $\sigma \propto \tau$, with τ the 1-particle lifetime due to electron-electron interactions. However the Umklapp processes do also provide a transport rate varying as T^2, so one often hears the not quite correct remark that the scattering rate in a Fermi liquid varies as T^2, therefore so does the resistivity ρ.

system. If, on the other hand, one found that $1/\tau$ were to scale precisely with $\max(\xi, T)$ (instead of $\max(\xi^2, T^2)$), the quasiparticles would be in a certain sense critically damped, i.e. not quite well defined, but not completely washed out either. This is what is frequently referred to as a "marginal Fermi liquid".[MFL]

2.3.7 Effective mass m^* of quasiparticles

Here I give a quick derivation of the relation between the Landau parameter F_{1s} which appears in the current and the effective mass m^*.

The net momentum of the volume V of quasiparticles is

$$\mathbf{P}_{qp} = 2V \sum_{\mathbf{k}} \mathbf{k} n_{\mathbf{k}}, \text{ net quasiparticle momentum} \tag{115}$$

also the total momentum of the Fermi liquid. Since the number of particles equals the number of quasiparticles, however, the quasiparticle and particle currents must also be equal

$$\mathbf{J}_{qp} = \mathbf{J}_p = 2V \sum_{\mathbf{k}} \mathbf{v}_{\mathbf{k}} n_{\mathbf{k}} \text{ net quasiparticle and particle current} \tag{116}$$

or, since the momentum is just the particle mass times this current

$$\mathbf{P}_p = 2Vm \sum_{\mathbf{k}} \mathbf{v}_{\mathbf{k}} n_{\mathbf{k}} \text{ net quasiparticle and particle momentum} \tag{117}$$

where $\mathbf{v}_{\mathbf{p}} = \nabla_k \tilde{\epsilon}_{\mathbf{k}}$, is the velocity of the quasiparticle. So

$$\sum_{\mathbf{k}} \mathbf{k} n_{\mathbf{k}} = m \sum_{\mathbf{k}} \nabla_k \tilde{\epsilon}_{\mathbf{k}} n_{\mathbf{k}} \tag{118}$$

Let's consider an arbitrary variation of $n_{\mathbf{k}}$, and remember that $\tilde{\epsilon}_{\mathbf{k}}$ depends on $n_{\mathbf{k}}$, so that

$$\delta\tilde{\epsilon}_{\mathbf{k}} = 2V \sum_{\mathbf{k}} f_{\mathbf{k},\mathbf{k}'} \delta n_{\mathbf{k}'} \,. \tag{119}$$

For Eq. 118, this means that

$$\begin{aligned} \sum_{\mathbf{k}} \mathbf{k} \delta n_{\mathbf{k}} &= m \sum_{\mathbf{k}} \nabla_k \tilde{\epsilon}_{\mathbf{k}} \delta n_{\mathbf{k}} \\ &\quad + m 2V \sum_{\mathbf{k}} \sum_{\mathbf{k}'} \nabla_{\mathbf{k}} \left(f_{\mathbf{k},\mathbf{k}'} \delta n_{\mathbf{k}'} \right) n_{\mathbf{k}} \,, \end{aligned} \tag{120}$$

or integrating by parts (and renaming $\mathbf{k} \to \mathbf{k}'$ in the last part), we get

$$\begin{aligned} \sum_{\mathbf{k}} \frac{\mathbf{k}}{m} \delta n_{\mathbf{k}} &= \sum_{\mathbf{k}} \nabla_k \tilde{\epsilon}_{\mathbf{k}} \delta n_{\mathbf{k}} \\ &\quad - 2V \int \sum_{\mathbf{k},\mathbf{k}'} \delta n_{\mathbf{k}} f_{\mathbf{k},\mathbf{k}'} \nabla_{\mathbf{k}'} n_{\mathbf{k}'} \,, \end{aligned} \tag{121}$$

The usual variational argument says that since $\delta n_{\mathbf{k}}$ is arbitrary, we must have that the integrands are equal

$$\frac{\mathbf{k}}{m} = \nabla_{\mathbf{k}} \tilde{\epsilon}_{\mathbf{k}} - 2V \sum_{\mathbf{k}'} f_{\mathbf{k},\mathbf{k}'} \nabla_{\mathbf{k}'} n_{\mathbf{k}'} \tag{122}$$

At $T = 0$ $\nabla_{\mathbf{k}'} n_{\mathbf{k}'} = -\hat{k}' \delta(k' - \mathbf{k}_F)$. The integral may now be evaluated by using the system isotropy in $\mathbf{k}$ space, and choosing $\mathbf{k}$ parallel $\hat{z}$. As we mostly concerned with Fermi surface properties we take $k = k_F$, and let θ be the angle between $\mathbf{k}$ (or the z-axis) and $\mathbf{k}'$, and finally note that on the Fermi surface $|\nabla_k \tilde{\epsilon}_k|_{k=k_F} = v_F = k_F/m^*$. Thus,

$$\frac{k_F}{m} = \frac{k_F}{m^*} + 2V \int \frac{k'^2 dk d\Omega}{(2\pi\hbar)^3} f_{\mathbf{k},\mathbf{k}'} \hat{k} \cdot \hat{k}' \delta(k' - k_F) \tag{123}$$

However, since both $\mathbf{k}$ and $\mathbf{k}'$ are restricted to the Fermi surface $\hat{k}' = \cos\theta$, and evaluating the integral over k, we get

$$\frac{1}{m} = \frac{1}{m^*} + 2Vk_F \int \frac{d\Omega}{(2\pi\hbar)^3} f_{\mathbf{k},\mathbf{k}'} \cos\theta \,, \tag{124}$$

If we now sum over (hidden) spins only the symmetric part of f appears

$$\frac{1}{m} \;=\; \frac{1}{m^*} + \frac{4\pi V k_F}{(2\pi\hbar)^3} \int d(\cos\theta)\, f^s(\theta) \cos\theta \,, \tag{125}$$

Now use decomposition (103), orthonormality of Legendre polynomials, and def. of Landau parameters:

$$\tag{126}$$

$$f^\alpha(\theta) \;=\; \sum_l f_l^\alpha P_l(\cos\theta) \,, \tag{127}$$

$$\int_{-1}^{1} dx P_n(x) P_m(x) dx \;=\; \frac{2}{2n+1}\delta_{nm} \tag{128}$$

$$N_0 f_l^\alpha \;=\; \frac{V m^* k_F}{\pi^2 \hbar^3} f_l^\alpha = F_l^\alpha \,, \tag{129}$$

we find that

$$\boxed{\frac{1}{m} = \frac{1}{m^*} + \frac{F_1^s}{3} \,,} \tag{130}$$

or $m^*/m = 1 + F_1^s/3$.

So effective mass and F_{1s} aren't independent, at least in a Galilean invariant system where (116) holds.